Testing New Conditioned Balance Equations by Simulating Turbulent Scalar Transport in Impinging Jet Flames

Andrei N. Lipatnikov

Department of Applied Mechanics Chalmers University of Technology

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Conditioned Balance Equations

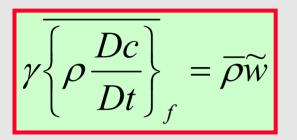
Combust. Flame **152** (2008) 529-547

$$\frac{\partial}{\partial t} (\overline{\rho} \widetilde{c}) + \frac{\partial}{\partial x_k} (\overline{\rho} \widetilde{c} \, \overline{u}_{kb}) = \gamma \overline{\left(\rho \frac{Dc}{Dt}\right)_f}$$

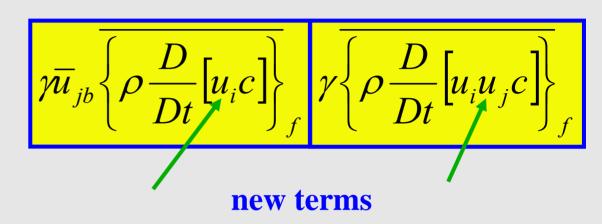
$$\frac{\partial}{\partial t} \left[\overline{\rho} \widetilde{c} \, \overline{u}_{ib} \right] + \frac{\partial}{\partial x_k} \left[\overline{\rho} \widetilde{c} \, \overline{u}_{ib} \overline{u}_{kb} \right] = -\frac{\partial}{\partial x_k} \left[\overline{\rho} \widetilde{c} \left(\overline{u_i' u_k'} \right)_b \right] - \overline{c} \left(\overline{\frac{\partial p}{\partial x_i}} \right)_b + \overline{c} \left(\overline{\frac{\partial \tau_{ik}}{\partial x_k}} \right)_b + \overline{c} \left(\overline{\frac{\partial \tau_{i$$

$$\begin{split} &\frac{\partial}{\partial t} \left[\overline{\rho} \widetilde{c} \left(\overline{u_i' u_j'} \right)_b \right] + \frac{\partial}{\partial x_k} \left[\overline{\rho} \widetilde{c} \, \overline{u_{kb}} \left(\overline{u_i' u_j'} \right)_b \right] + \overline{\rho} \widetilde{c} \left(\overline{u_i' u_k'} \right)_b \frac{\partial \overline{u_{jb}}}{\partial x_i} + \overline{\rho} \widetilde{c} \left(\overline{u_j' u_k'} \right)_b \frac{\partial \overline{u_{ib}}}{\partial x_i} \\ &= - \frac{\partial}{\partial x_k} \left[\overline{\rho} \widetilde{c} \left(\overline{u_i' u_j' u_k'} \right)_b \right] - \overline{c} \left[\overline{u_j'} \frac{\partial p}{\partial x_i} \right)_b - \overline{c} \left[\overline{u_i'} \frac{\partial p}{\partial x_j} \right]_b + \overline{c} \left[\overline{u_j'} \frac{\partial \tau_{ik}}{\partial x_k} \right)_b + \overline{c} \left[\overline{u_i'} \frac{\partial \tau_{jk}}{\partial x_k} \right)_b \\ &+ \gamma \left\{ \overline{\rho} \frac{D}{Dt} \left[u_i u_j c \right] \right\}_f - \gamma \overline{u_{jb}} \left\{ \overline{\rho} \frac{D}{Dt} \left[u_i c \right] \right\}_f - \gamma \overline{u_{ib}} \left\{ \overline{\rho} \frac{D}{Dt} \left[u_j c \right] \right\}_f + \gamma \overline{u_{ib}} \overline{u_{jb}} \left\{ \overline{\rho} \frac{Dc}{Dt} \right\}_f \end{split}$$

Flamelet Terms: A Key Issue



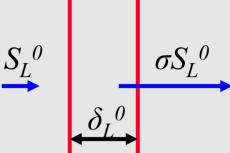
addressed by many models



If the new terms may be closed using a submodel for the mean reaction rate, then the conditioned balance equations substantially facilitate modeling of the effects of a premixed flame on turbulent flow.

The Simplest Closure

If flamelet structure is assumed to be unperturbed by turbulent eddies, then



$$\overline{\left(\rho \frac{Dq}{Dt}\right)_{f}} = \rho_{u} S_{L}^{0} \int_{\varepsilon}^{1-\varepsilon} \frac{dq}{dx} P_{f}(c) dc = \rho_{u} S_{L}^{0} \int_{\varepsilon}^{1-\varepsilon} \frac{dq}{dx} \left(\frac{dc}{dx}\right)^{-1} \frac{dc}{\delta_{L}^{0}} = \frac{\rho_{u} S_{L}^{0}}{\delta_{L}^{0}} (q_{b} - q_{u})$$

$$\overline{\rho}\widetilde{w} = \gamma \overline{\left(\rho \frac{Dc}{Dt}\right)_{f}} = \gamma \frac{\rho_{u} S_{L}^{0}}{\delta_{L}^{0}}$$

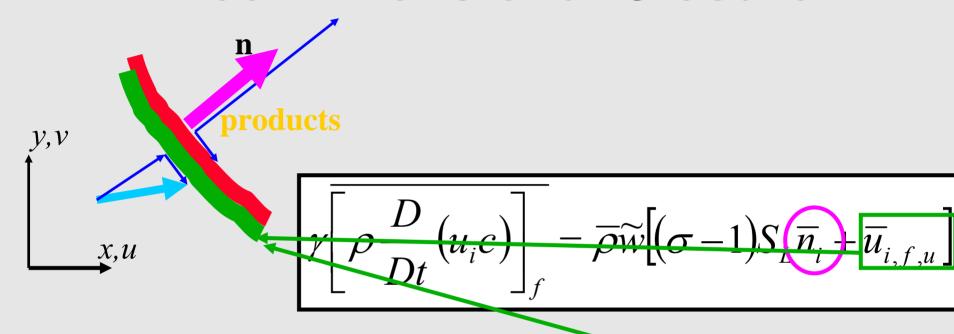
$$\gamma \overline{\left[\rho \frac{D}{Dt}(uc)\right]_{f}} = \gamma \frac{\rho_{u} S_{L}^{0}}{\delta_{L}^{0}} \sigma S_{L}^{0}$$

$$\gamma \overline{\left[\rho \frac{D}{Dt}(u^{2}c)\right]_{f}} = \gamma \frac{\rho_{u} S_{L}^{0}}{\delta_{L}^{0}} (\sigma S_{L}^{0})^{2}$$

$$\gamma \overline{\left[\rho \frac{D}{Dt}(uc)\right]_f} = \sigma S_L^0 \overline{\rho} \widetilde{w}$$

 $\gamma \left[\rho \frac{D}{Dt} (u^2 c) \right]_f = (\sigma S_L^0)^2 \, \overline{\rho} \widetilde{w}$

Three-Dimensional Closure

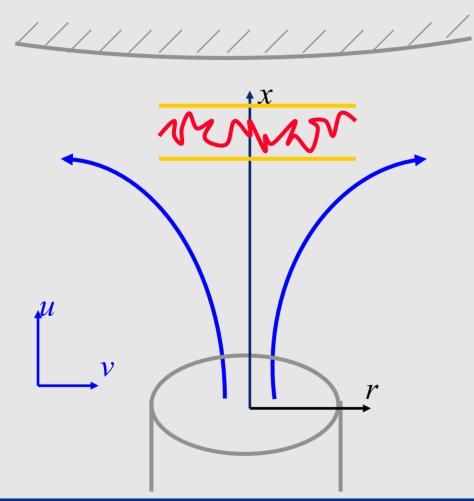


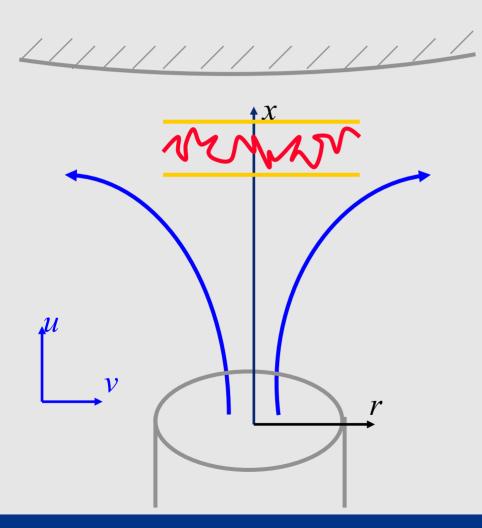
$$\gamma \left[\overline{\rho} \frac{D}{Dt} (u_i u_j c) \right]_f = \overline{\rho} \widetilde{w} \left[\overline{n_i n_j} \mathcal{S}_{i,j} (\sigma - 1)^2 S_L^2 + \left(\overline{n_i u_{j,f,u}} + \overline{n_j u_{i,f,u}} \right) (\sigma - 1) S_L + \left(\overline{u_i u_j} \right)_{f,u} \right]$$

The goal of the present work is

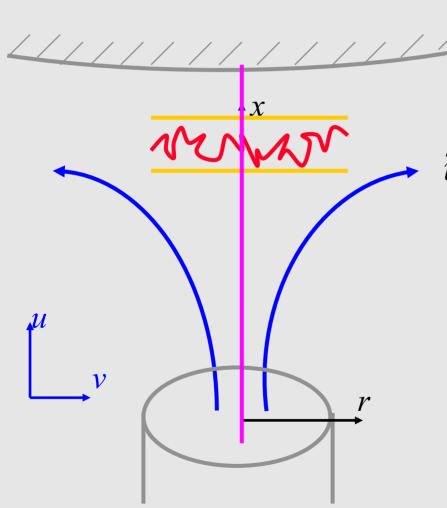
- to perform the first test of the conditioned balance equations and
- to show that they are able to facilitate modeling the effects of premixed flame on turbulent flow.

Premixed Turbulent Stagnation Flame Stabilized in an Impinging Jet





1. Strong effect of combustion on scalar transport

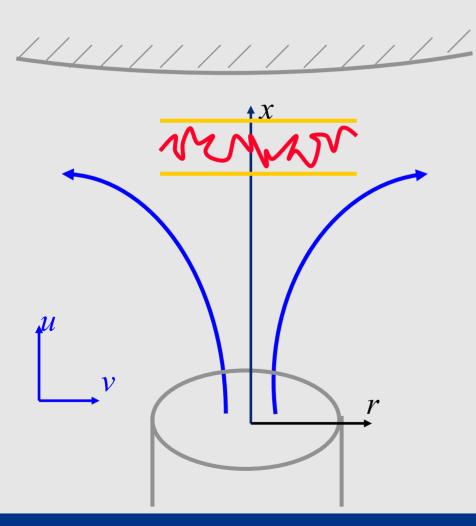


- 1. Strong effect of combustion on scalar transport
- 2. Quick simulations

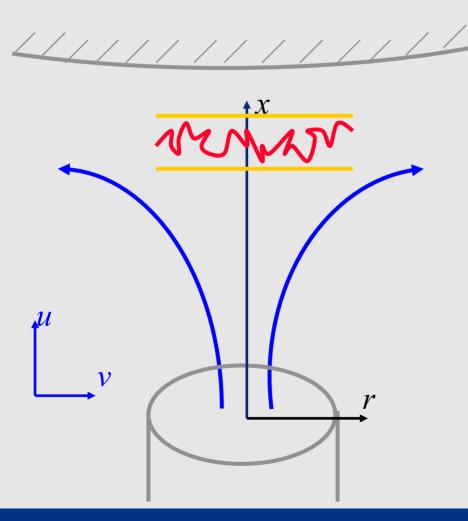
$$\widetilde{u}(x,r) \approx \widetilde{u}(x)$$
 $\widetilde{c}(x,r) \approx \widetilde{c}(x)$

$$\frac{\partial \widetilde{v}}{\partial r}(x,0) = 0 \quad \widetilde{v}(x,r) \approx r\widetilde{g}(x)$$

$$\frac{\frac{d}{dx}(\bar{\rho}\tilde{u}) + 2\bar{\rho}\tilde{g} = 0;}{\frac{d}{dx}(\bar{\rho}\tilde{u}\tilde{g}) + 3\bar{\rho}\tilde{g}^{2} = \frac{Q}{\rho_{u}U_{1}^{2}}}$$



- 1. Strong effect of combustion on scalar transport
- 2. Quick simulations
- 3. Target-directed, "pure" test

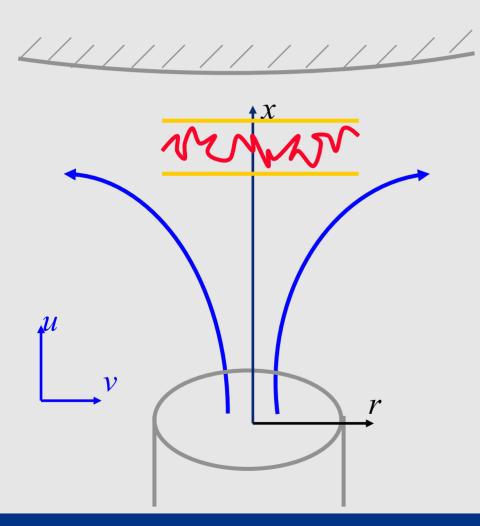


- 1. Strong effect of combustion on scalar transport
- 2. Quick simulations
- 3. Target-directed, "pure" test
- 4. Representative test
- > Cho et al. (1988)
- Cheng & Shepherd (1991)
- *▶Li et al. (1994)*
- ➤ Stevens et al. (1998)

Conditions of Measurements and Simulations

d	U_{I}	Fuel	Ф	S_L	σ	u'/S_L	Flame
m	m/s			m/s			
0.075	5	CH ₄	1.0	0.37	7.51	1.23	#1 Cho et al.
0.1	5	C_2H_6	1.0	0.76	8.00	0.53	S9 Cheng & Shepherd
0.03	3.6	CH ₄	0.89	0.31	7.08	0.70	h4 Li et al.
0.03	3.6	CH ₄	0.89	0.31	7.08	0.70	h6 Li et al.
0.035	0.75	CH ₄	0.6	0.085	5.54	0.71	set 1 Stevens et al.
0.035	3	CH ₄	1.0	0.37	7.51	0.90	set 2 Stevens et al.
0.035	2.25	CH ₄	1.3	0.21	7.11	0.85	set 3 Stevens et al.

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- 1. Strong effect of combustion on scalar transport
- 2. Quick simulations
- 3. Target-directed, "pure" test
- 4. Representative test
- 5. Challenge
- Cheng & Shepherd (1991)
- *▶Li et al. (1994)*
- ➤ Stevens et al. (1998)
- > Cho et al. (1988)

Main Goal of Simulations

To validate the conditioned balance equations

$$\frac{\partial}{\partial t} \left[\overline{\rho} (1 - \widetilde{c}) \right] + \frac{\partial}{\partial x_k} \left[\overline{\rho} (1 - \widetilde{c}) \overline{u}_{ku} \right] = -\gamma \left[\overline{\rho} \frac{Dc}{Dt} \right]_f$$

$$\frac{\partial}{\partial t} \left(\overline{\rho} \widetilde{c} \right) + \frac{\partial}{\partial x_k} \left(\overline{\rho} \widetilde{c} \, \overline{u}_{kb} \right) = \gamma \left[\overline{\rho} \frac{Dc}{Dt} \right]_f$$

$$\frac{\partial}{\partial t} (\overline{\rho} \widetilde{c}) + \frac{\partial}{\partial x_k} (\overline{\rho} \widetilde{c} \, \overline{u}_{kb}) = \gamma \left(\rho \frac{Dc}{Dt} \right)$$

$$\frac{\partial}{\partial t} \left[\overline{\rho} (1 - \overline{c}) \overline{u}_{iu} \right] + \frac{\partial}{\partial x_k} \left[\overline{\rho} (1 - \overline{c}) \overline{u}_{iu} \overline{u}_{ku} \right] = -\frac{\partial}{\partial x_k} \left[\overline{\rho} (1 - \overline{c}) (\overline{u_i' u_k'})_u \right] - (1 - \overline{c}) \left(\frac{\partial p}{\partial x_i} \right)_u + (1 - \overline{c}) \left(\frac{\partial r_{ik}}{\partial x_k} \right)_u + \gamma \left\{ \overline{\rho} \frac{D}{Dt} \left[u_i (1 - c) \right] \right\}_f$$

$$\frac{\partial}{\partial t} \left[\overline{\rho} \widetilde{c} \, \overline{u}_{ib} \right] + \frac{\partial}{\partial x_k} \left[\overline{\rho} \widetilde{c} \, \overline{u}_{ib} \overline{u}_{kb} \right] = -\frac{\partial}{\partial x_k} \left[\overline{\rho} \widetilde{c} \left(\overline{u'_i u'_k} \right)_b \right] - \overline{c} \left(\frac{\partial p}{\partial x_i} \right)_b + \overline{c} \left(\frac{\partial \tau_{ik}}{\partial x_k} \right)_k + \gamma \overline{\left\{ \rho \frac{D}{Dt} \left[u_i c \right] \right\}}_f$$

supplemented with the simplest closure of flamelet terms

$$\boxed{\gamma \left[\rho \frac{Du_i}{Dt} \right]_f} = \overline{\rho} \widetilde{w} (\sigma - 1) S_L \overline{n}$$

$$\boxed{\gamma \boxed{\rho \frac{Du_i}{Dt}}_f = \overline{\rho} \widetilde{w} (\sigma - 1) S_L \overline{n}} \boxed{\gamma \boxed{\rho \frac{D}{Dt} (u_i c)}_f = \overline{\rho} \widetilde{w} [(\sigma - 1) S_L \overline{n}_i + \overline{u}_{i,f,u}]}$$

by simulating countergradient scalar transport

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Key Equation

turbulent diffusion

$$\frac{1}{2} \frac{d}{d\zeta} \left(\overline{u}_{b}^{2} - \overline{u}_{u}^{2} \right) = -\sigma \overline{\rho} \left[\left(\frac{dp}{d\zeta} \right)_{b} - \left(\frac{dp}{d\zeta} \right)_{u} \right] - (\sigma - 1) \frac{d\overline{p}}{d\zeta} + (\sigma - 1) S_{L} \overline{n}_{x} \frac{\Omega}{\widetilde{c}} - \left(\sigma \frac{\overline{u}_{b} - \overline{u}_{f,u}}{\overline{c}} - \frac{\overline{u}_{u} - \overline{u}_{f,u}}{1 - \overline{c}} \right) \Omega$$

$$\zeta \equiv \frac{x}{d}$$

$$\overline{\rho u''c''} \approx \overline{\rho}\widetilde{c}(1-\widetilde{c})(u_b-u_u)$$

$$\Omega \equiv \frac{d}{\rho_{u}U_{1}} \, \overline{\rho} \widetilde{w}$$

Closure I: Difference in **Conditioned Pressure Gradients**

$$P(t, \vec{x}, q) = (1 - \overline{c})\delta(q - q_u) + \gamma(t, \vec{x})P_f(t, \vec{x}, q) + \overline{c}\delta(q - q_b)$$

$$\overline{c'\nabla p'} - \gamma \overline{(c'\nabla p')}_f = \overline{c}(1 - \overline{c}) \overline{(\nabla p)}_b - \overline{(\nabla p)}_u$$

Inert constant-density flows:

$$\overline{c}(1-\overline{c})[(\overline{\nabla p})_{b}-(\overline{\nabla p})_{u}]=\overline{c'\nabla p'}=-C_{1}\frac{\overline{\varepsilon}}{\overline{l_{r}}}\overline{\mathbf{u'}c'}=C_{2}\overline{k}_{u}\nabla\overline{c}$$

non-reacting terms

$$= -C_1 \frac{\overline{\varepsilon}}{\overline{k}} \mathbf{u}' c' = C_2 \overline{k}_u \nabla \overline{c}$$

gradient diffusion closure

Launder's

closure

$$\overline{c}(1-\overline{c})[(\overline{\nabla p})_b - (\overline{\nabla p})_u] = C_2 \overline{\rho} \overline{k}_u \nabla \widetilde{c} \quad C_2 \approx \frac{1}{2}$$

Key Equation

turbulent diffusion

mean pressure gradient

$$\left| \frac{1}{2} \frac{d}{d\zeta} \left(\overline{u}_b^2 - \overline{u}_u^2 \right) = -\sigma \overline{\rho} \left[\left(\frac{dp}{d\zeta} \right)_b - \left(\frac{dp}{d\zeta} \right)_u \right] - (\sigma - 1) \frac{d\overline{p}}{d\zeta}$$

$$+(\sigma-1)S(\overline{n}_{x})\frac{\Omega}{\widetilde{c}}-\left(\sigma\frac{\overline{u}_{b}-(\overline{u}_{f,u})}{\overline{c}}-\frac{\overline{u}_{u}-\overline{u}_{f,u}}{1-\overline{c}}\right)\Omega$$

flamelet terms

$$\zeta \equiv \frac{x}{d}$$

$$\overline{\rho u''c''} \approx \overline{\rho}\widetilde{c}(1-\widetilde{c})(u_b-u_u)$$

$$\Omega \equiv \frac{d}{\rho_u U_1} \overline{\rho} \widetilde{w}$$

Closure II: Flamelet Normal

Experimental data obtained by Chen & Bilger (2002) from a number of Bunsen-type premixed turbulent flames show that the projection of the averaged normal vector to flamelets on the line perpendicular to the mean flame brush is close to 2/3.



$$\overline{n}_x = -\frac{2}{3}$$

Key Equation

turbulent diffusion

mean pressure gradient

$$\frac{1}{2} \frac{d}{d\zeta} \left(\overline{u}_b^2 - \overline{u}_u^2 \right) = -\sigma \overline{\rho} \left[\left(\frac{dp}{d\zeta} \right)_b - \left(\frac{dp}{d\zeta} \right)_u \right] - (\sigma - 1) \frac{d\overline{p}}{d\zeta}$$

$$+(\sigma-1)S_{L}^{\prime}\overline{n}_{x}\frac{\Omega}{\widetilde{c}}-\left(\sigma\frac{\overline{u}_{b}-(\overline{u}_{f,u})}{\overline{c}}-\frac{\overline{u}_{u}-\overline{u}_{f,u}}{1-\overline{c}}\right)\Omega_{L}^{\prime}$$

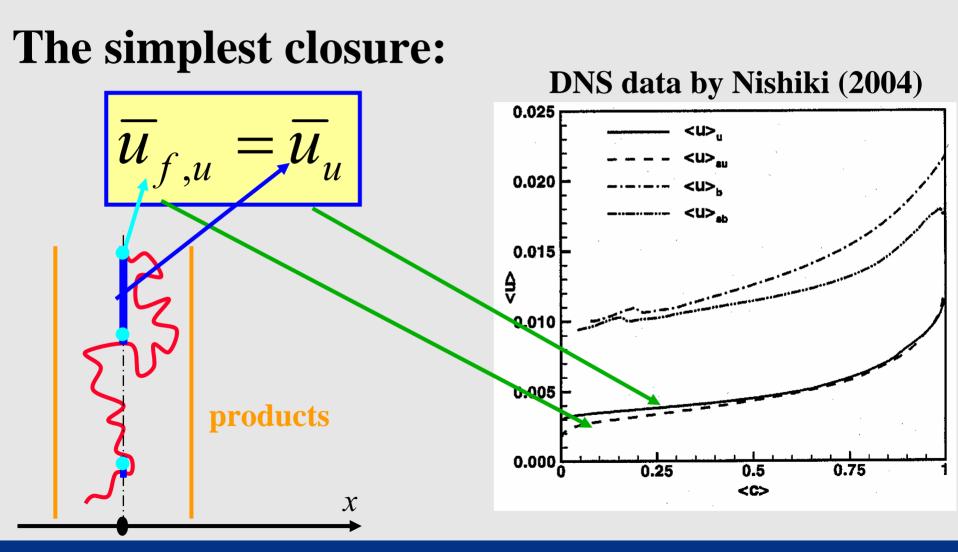
flamelet terms

$$\zeta \equiv \frac{x}{d}$$

$$\overline{\rho u''c''} \approx \overline{\rho}\widetilde{c}(1-\widetilde{c})(u_b-u_u)$$

$$\Omega \equiv \frac{d}{\rho_{u}U_{1}} \overline{\rho} \widetilde{w}$$

Closure III: Velocity Ahead Flamelets



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Key Equation

turbulent diffusion

mean pressure gradient

$$\frac{1}{2} \frac{d}{d\zeta} \left(\overline{u}_b^2 - \overline{u}_u^2 \right) = -\sigma \overline{\rho} \left[\frac{dp}{d\zeta} \right]_b - \left(\frac{dp}{d\zeta} \right)_u - (\sigma - 1) \frac{d\overline{p}}{d\zeta}$$

$$+(\sigma-1)S_{L}^{\prime}\overline{n}_{x}\frac{\Omega}{\widetilde{c}}-\left(\sigma\frac{\overline{u}_{b}-\overline{u}_{f,u}}{\overline{c}}-\frac{\overline{u}_{u}-\overline{u}_{f,u}}{1-\overline{c}}\right)\Omega$$

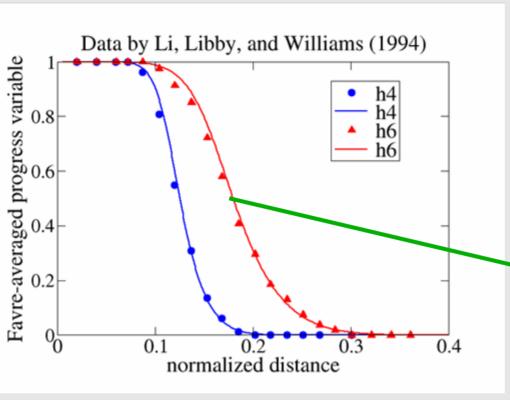
flamelet terms

$$\zeta \equiv \frac{x}{d}$$

$$\overline{\rho u''c''} \approx \overline{\rho}\widetilde{c}(1-\widetilde{c})(u_b-u_u)$$

$$\Omega \equiv \frac{d}{\rho_{u}U_{1}} \overline{\rho} \widetilde{w}$$

Closure IV: Mean Reaction Rate



$$\overline{c} = \frac{1}{2}\operatorname{erfc}(\xi\sqrt{\pi}) = \frac{1}{\sqrt{\pi}} \int_{\xi\sqrt{\pi}}^{\infty} e^{-\varsigma^2} d\varsigma;$$

Combustion progress variable balance equation:

$$\Omega = \frac{d}{d\zeta} (\overline{\rho}\widetilde{u}\widetilde{c}) + 2\overline{\rho}\widetilde{g}\widetilde{c}$$

$$+ \frac{d}{d\zeta} [\overline{\rho}\widetilde{c}(1 - \widetilde{c})(\overline{u}_b - \overline{u}_u)]$$

$$+ 2\overline{\rho}\widetilde{c}(1 - \widetilde{c})(\widetilde{g}_b - \widetilde{g}_u)$$

Closed Key Equations

$$\frac{1}{2} \frac{d}{d\zeta} \left(\overline{u}_{b}^{2} - \overline{u}_{u}^{2} \right) = -\frac{3}{4} \frac{\sigma \overline{\rho}^{2} u'^{2} \cdot d\overline{c}}{\overline{c} (1 - \overline{c})} \frac{d\overline{c}}{d\zeta}
- (\sigma - 1) \frac{d\overline{p}}{d\zeta} - \left[\frac{2}{3} \overline{\rho} (\sigma - 1) S_{L} - (\overline{u}_{u} - \overline{u}_{b}) \right] \frac{\sigma \Omega}{\overline{c}}$$

$$\Omega = \frac{d}{d\zeta} (\overline{\rho}\widetilde{u}\widetilde{c}) + \frac{d}{d\zeta} [\overline{\rho}\widetilde{c}(1-\widetilde{c})(\overline{u}_b - \overline{u}_u)]
+ 2\overline{\rho}\widetilde{g}\widetilde{c} + 2\overline{\rho}\widetilde{c}(1-\widetilde{c})(\widetilde{g}_b - \widetilde{g}_u)$$

Other Equations

Mass:
$$\frac{d}{d\mathcal{E}}(\bar{\rho}\tilde{u}) + 2\bar{\rho}\tilde{g} = 0;$$

Radial velocity:
$$\frac{d}{d\zeta} (\bar{\rho} \tilde{u} \tilde{g}) + 3\bar{\rho} \tilde{g}^2 = Q;$$

Axial velocity:
$$\frac{d}{d\zeta} \left(\overline{\rho} \widetilde{u}^2 \right) + \frac{d}{d\zeta} \left[\overline{\rho} \widetilde{c} \left(1 - \widetilde{c} \right) \left(\overline{u}_b - \overline{u}_u \right)^2 \right] + 2 \overline{\rho} \widetilde{u} \widetilde{g} = -\frac{d\overline{\rho}}{d\zeta};$$

BML state equation:
$$\rho_b \overline{c} = \overline{\rho} \widetilde{c} = \frac{\widetilde{c}}{1 + (\sigma - 1)\widetilde{c}}$$

Boundary conditions:
$$\widetilde{u}(1) = -1$$
; $\widetilde{g}(1) = g_1$; $\overline{u}_b(\zeta_1) = \overline{u}_u(\zeta_1)$

Parameters Q and g_I were adjusted by comparing the measured and computed mean axial velocities within flame brush.

Target-Directed Test

$$\rho_{b}\overline{c} = \overline{\rho}\widetilde{c} = \frac{\widetilde{c}}{1 + (\sigma - 1)\widetilde{c}}$$

$$\frac{1}{2} \frac{d}{d\zeta} (\overline{u_{b}^{2}} - \overline{u_{u}^{2}}) = -\frac{3}{4} \frac{\sigma \overline{\rho}^{2} u'^{2}}{\overline{e}(1 - \overline{c})} \frac{d\widetilde{c}}{d\zeta}$$

$$-(\sigma - 1) \frac{d\overline{p}}{d\zeta} - \frac{2}{3} \overline{\rho}(\sigma - 1) \mathcal{S}_{L} - (\overline{u_{u}} - \overline{u_{b}}) \frac{\sigma}{c}$$

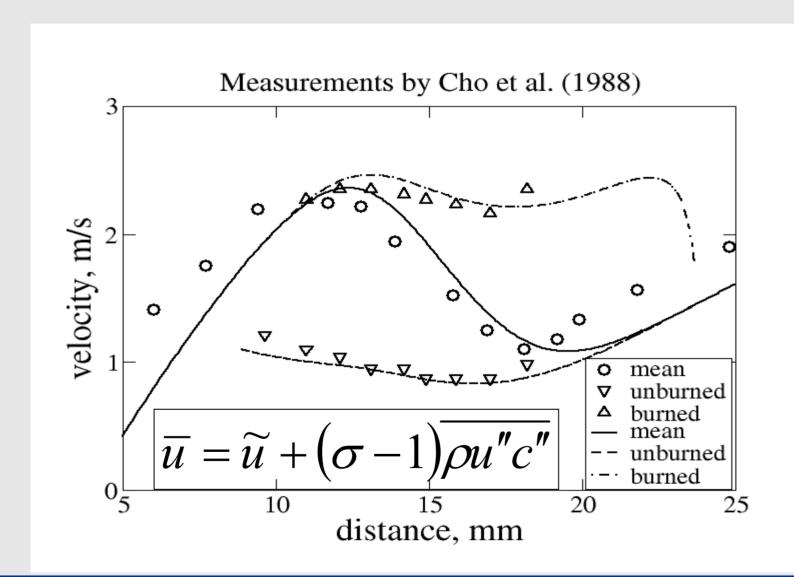
$$\frac{d}{d\zeta} (\overline{\rho}\widetilde{u}^{2}) + \frac{d}{d\zeta} [\overline{\rho}\widetilde{c}(1 - \widetilde{c})(\overline{u_{b}} - \overline{u_{u}})^{2}] + 2\overline{\rho}\widetilde{u}\widetilde{g} = -\frac{d\overline{p}}{d\zeta}; \qquad \Omega = \frac{d}{d\zeta} (\overline{\rho}\widetilde{u}\widetilde{c}) + \frac{d}{d\zeta} [\overline{\rho}\widetilde{c}(1 - \widetilde{c})(\overline{u_{b}} - \overline{u_{u}})]$$

$$+2\overline{\rho}\widetilde{g}\widetilde{c} + 2\overline{\rho}\widetilde{c}(1 - \widetilde{c})(\widetilde{g}_{b} - \widetilde{g}_{u})$$

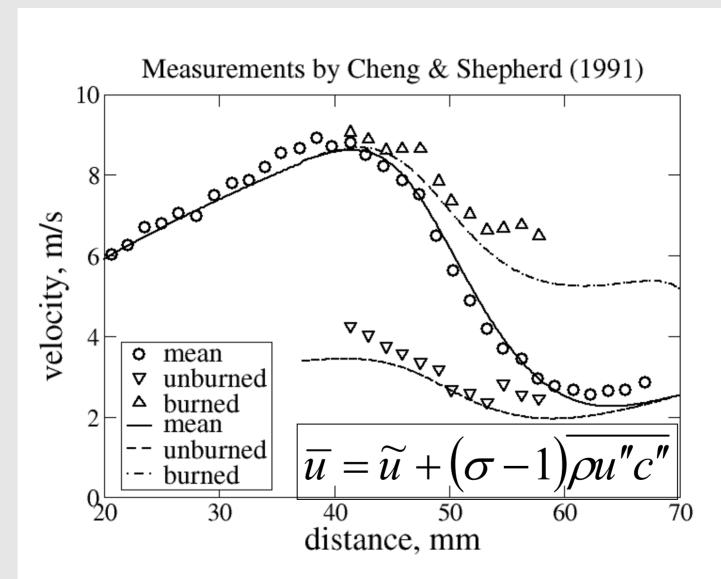
$$\frac{d}{d\zeta} (\overline{\rho}\widetilde{u}) + 2\overline{\rho}\widetilde{g} = 0;$$

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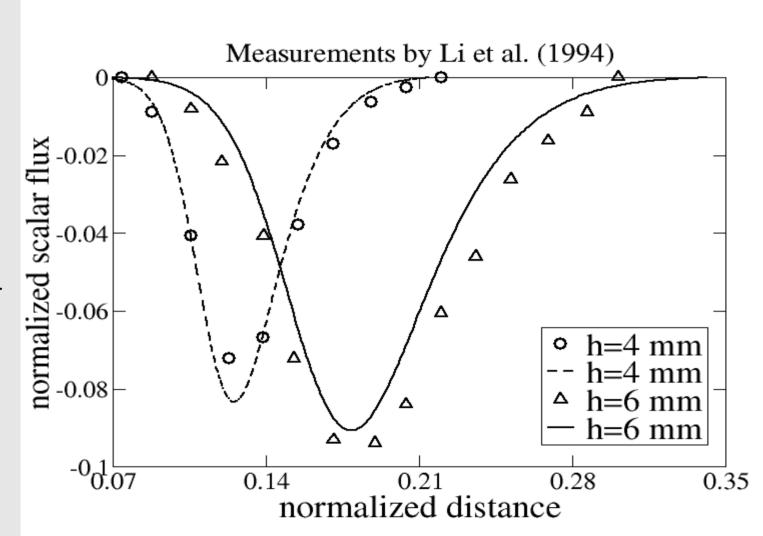
Validation



Validation II

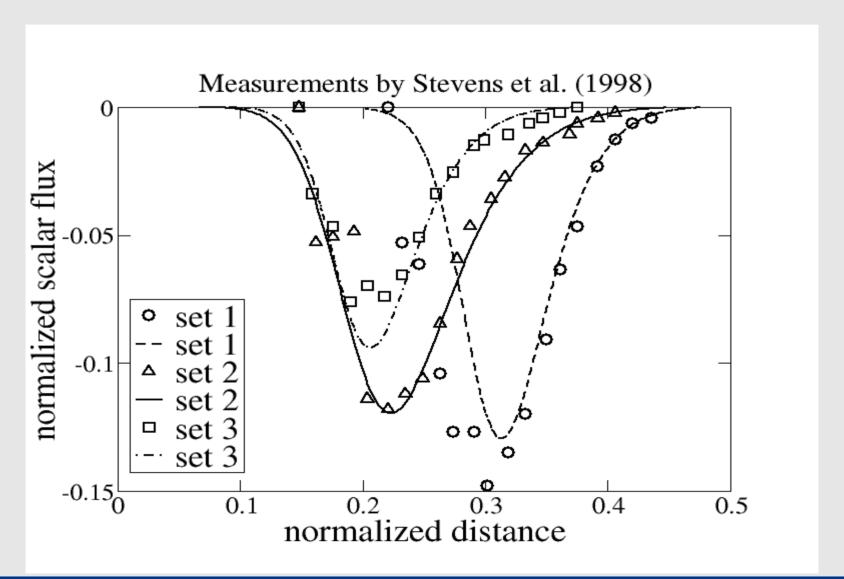


Validation III

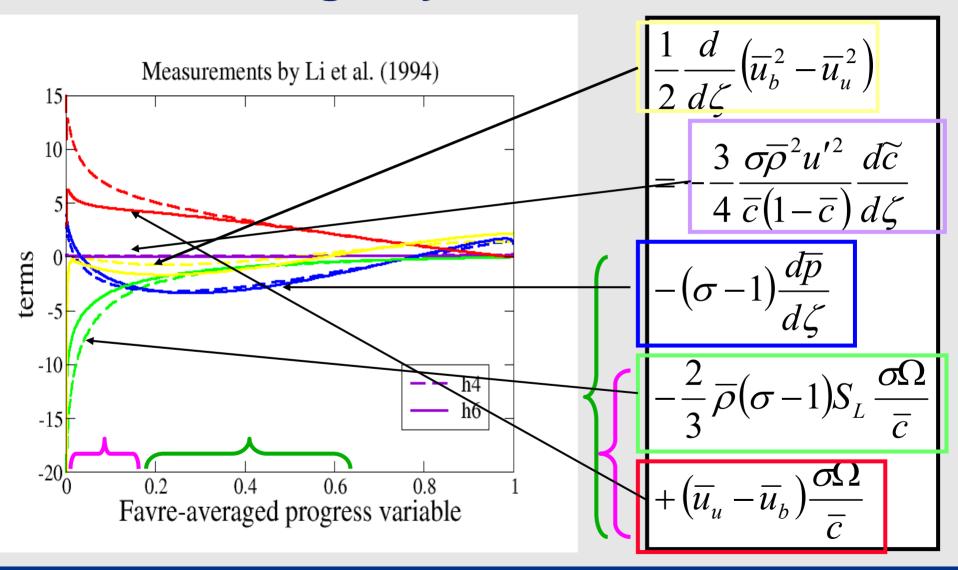


 $\frac{\overline{\rho u''c''}}{\overline{\rho}U_1}$

Validation IV



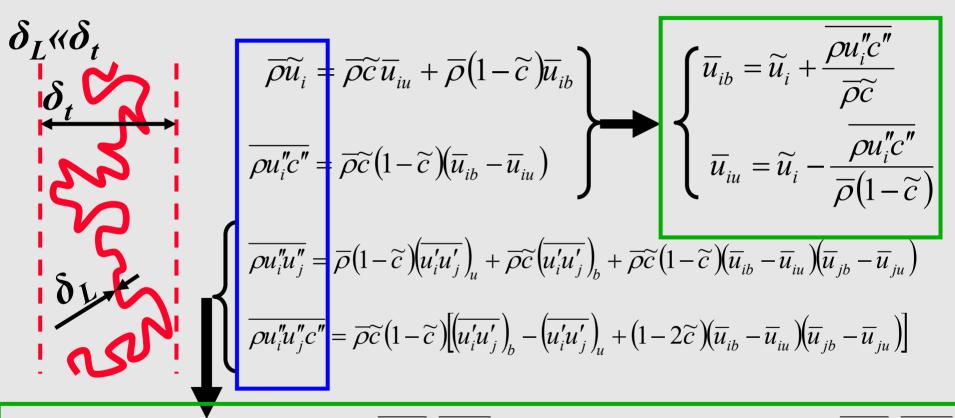
Governing Physical Mechanisms



Main Message

The proposed approach is promising!

Balance Equations for Conditioned Second Moments I



$$\overline{\rho}(1-\widetilde{c})(\overline{u_i'u_j'})_u = (1-\widetilde{c})\overline{\rho u_i''u_j''} - \overline{\rho u_i''u_j''c''} - \frac{\rho u_i''c'' \cdot \rho u_j''c''}{\overline{\rho}(1-\widetilde{c})} \qquad \overline{\rho}\widetilde{c}(\overline{u_i'u_j'})_b = \widetilde{c}\overline{\rho u_i''u_j''} + \overline{\rho u_i''u_j''c''} - \frac{\rho u_i''c'' \cdot \rho u_j''c''}{\overline{\rho}\widetilde{c}}$$